

Surface-induced disorder and aperiodic perturbations at first-order transitions

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In systems displaying a bulk first-order transition the order parameter may vanish continuously at a free surface, a phenomenon which is called *surface-induced disorder*. In the presence of surface-induced disorder the correlation lengths, parallel and perpendicular to the surface, diverge at the bulk transition point. In this way the surface induces an anisotropic power-law singular behavior for some bulk quantities. For example, in a finite system of transverse linear size L , the response functions diverge as $L^{(d-1)z+1}$, where d is the dimension of the system and z is the anisotropy exponent. We present a general scaling picture for this *anisotropic discontinuity fixed point*. Our phenomenological results are confronted with analytical and numerical calculations on the two-dimensional q -state Potts model in the large- q limit. The scaling results are demonstrated to apply also for the same model with a layered, Fibonacci-type modulation of the couplings for which the anisotropy exponent is a continuous function of the strength of the quasiperiodic perturbation.

I. INTRODUCTION

At a first-order phase transition several physical quantities, such as the order parameter and the energy density, have a discontinuous behavior in the bulk and the correlation lengths remain generally finite. In spite of the absence of a diverging “true” length scale in the problem, a successful scaling theory for first-order transitions has been developed,^{1,2} with scaling exponents such as

$$\beta_D = 0, \quad \alpha_D = \gamma_D = 1, \quad \delta_D = \infty, \quad (1.1)$$

which are compatible with discontinuities. The divergent length scale appearing in the scaling theory is associated with the persistence length of the coexisting phases,² behaving as $|t|^{-\nu_D}$ ($|h|^{-\nu_D^h}$) for a temperature (field) deviation from the transition point, with critical exponents

$$\nu_D = 1/d, \quad \nu_D^h = 1/d, \quad (1.2)$$

where d denotes the dimension of the system. In the renormalization group analysis of specific models, first-order transitions have been identified,^{1,3,4} which are controlled by a so-called discontinuity fixed point (DFP) with thermal and magnetic scaling dimensions $y_t = \ln \Lambda_t / \ln b = d$ and $y_h = \ln \Lambda_h / \ln b = d$. These dimensions are compatible with the value of ν_D and ν_D^h in Eq. (1.2) whereas other scaling exponents in Eq. (1.1) follow from scaling and hyperscaling relations.

For a system with a free surface at a bulk first-order transition two diverging lengths can be identified, ξ_{\parallel} associated with the correlations in the direction parallel to the surface and ξ_{\perp} in the perpendicular direction.

Due to missing bonds, the surface is more weakly coupled than the bulk. As a consequence, the surface order parameter vanishes continuously at the bulk transition point. This phenomenon, called *surface-induced disorder*⁵ (SID), is closely related to wetting phenomena.⁶ It has been studied using mean-field theory^{7,8} and Monte Carlo simulations⁹ and has been observed in some experimental systems.¹⁰ For the two-dimensional (2D) Potts model exact results have been obtained in the large- q limit and the universality of the critical and tricritical exponents in the bulk first-order transition regime, $q > 4$, has been accurately demonstrated by density matrix renormalization calculations.¹¹

The presence of diverging length scales in the problem suggests a possible scaling behavior for singular quantities, both at the surface and in the bulk of the system. Here we notice two peculiarities concerning the bulk scaling relations. First, in the geometry with a free surface there is an inherent anisotropy in the problem since the two length scales are related by

$$\xi_{\parallel} \sim \xi_{\perp}^z, \quad (1.3)$$

with an anisotropy exponent z which is generally greater than 1. Consequently, scaling for SID is strongly anisotropic in contrast to the original DFP theory, which was developed for isotropic scaling in the bulk.² Our second remark concerns the behavior of the system as the thermodynamic limit is approached. In a system of linear size L , the disordering effect of the surface in the bulk is limited to a temperature range $\Delta t \sim L^{-1/\nu_{\perp}}$ around the critical temperature, where ν_{\perp} is the perpendicular correlation length exponent [see below in Eq. (2.2)]. In the thermodynamic limit, when $L \rightarrow \infty$, the SID is present

in the bulk just at the transition point, when the scaling functions are singular, having either a jump or δ -function-like singularities. In a finite system, however, the scaling functions behave regularly, so that one has a “true” finite-size scaling behavior, which is measurable, for the specific heat or the susceptibility at the transition point.

Another problem of theoretical interest at a first-order transition point accompanied by SID is the influence of different types of perturbations, such as localized or extended defects,¹² quenched disorder,¹³ etc., on the bulk and surface transitions. Here we mainly consider the effect of a quasiperiodic or, more generally, aperiodic modulation of the couplings in the bulk. The influence of such perturbations on order-disorder phase transitions has been studied in detail for the Ising model,¹⁴ in particular in 2D with a layered structure (i.e., when the aperiodic perturbation has a 1D variation) and in the related quantum Ising spin chains. Among others, for marginal aperiodic sequences, coupling-dependent anisotropic critical behavior has been found.^{15–17}

At a first-order transition point, such as for the 2D Potts model with $q > 4$,^{18,19} the relevance or irrelevance of the effect of aperiodic perturbations is unclear. One can use an analogy with the rigorous result of Aizenman and Wehr,²⁰ stating that in 2D a first-order transition always softens into a second-order one, due to quenched disorder. Such a softening of the transition was indeed observed in a Monte Carlo study of the 2D Potts model with $q > 4$ for some types of layered aperiodic perturbations.²¹ However, due to computational difficulties, quantitative results about the phase transitions, such as critical exponents, could not be obtained.

In the present paper we use another approach to study the effect of aperiodic perturbations at a first-order transition point and to obtain quantitative results. For this purpose we consider the 2D Potts model¹⁹ on layered lattices and take the extreme anisotropic limit,²² when the logarithm of the transfer matrix of the model corresponds to the Hamiltonian of an aperiodic quantum Potts chain. Then we consider the large- q limit of the model, for which a consistent $1/\sqrt{q}$ expansion is defined and the leading term can be treated by analytical or very efficient numerical methods. In analogy with the results on the marginal quantum Ising chains, one expects that with marginal perturbations the critical exponents, in particular the anisotropy exponent, become coupling dependent. Indeed, with a Fibonacci-type modulation of the couplings, which is related to the 2D Penrose quasilattice, we have found continuously varying anisotropic scaling. In this way we have obtained a more general testing ground for the scaling relations in the presence of SID.

The structure of the paper is the following. In Sec. II we present the phenomenological scaling theory for SID both in the bulk and at the surface. In Sec. III we introduce the quantum Potts model and its representation in the large- q limit. In Sec. IV solutions of the model on

the regular lattice and on the Fibonacci quasilattice are confronted with predictions of the SID scaling picture. The results are discussed in Sec. V.

II. SCALING BEHAVIOR WITH SURFACE-INDUCED DISORDER

We consider a d -dimensional (magnetic) system in the slab geometry with two surfaces at a large finite distance L apart, whereas the extent of the system is infinite in the other $(d-1)$ dimensions, parallel to the surface. The system displays a bulk first-order transition and has q degenerate ordered phases. The state of the system on the surface at $l = L$ is fixed into one of these phases (by applying a local magnetic field in the appropriate direction) whereas the other surface at $l = 1$ is free. The temperature t is measured relative to the transition point and a bulk ordering (magnetic) field of strength h is applied. Due to the disordering effect of missing bonds, the order parameter profile m_l is monotonically decreasing towards the free surface. The surface order parameter m_1 may behave in two qualitatively different ways as the temperature is increased to the transition point. Either m_1 , like the bulk order parameter $m_b = m_{L/2}$, has a finite jump at $t = 0$ (first-order surface transition) or—and this is the case considered below— m_1 vanishes continuously as

$$m_1 \sim (-t)^{\beta_1}, \quad t < 0, \quad (2.1)$$

with a surface magnetization exponent β_1 (second-order surface transition). In this case the extent of the surface region ξ_\perp , where $m_l \sim m_1$ ($1 < l < \xi_\perp$), is diverging at the transition point as

$$\xi_\perp \sim (-t)^{-\nu_\perp}. \quad (2.2)$$

As mentioned in the Introduction, this phenomenon associated with the long-distance disordering effect of a free surface is called SID.

In the region of SID, correlations between spins in the direction parallel to the free surface decay exponentially, which defines a new correlation length ξ_\parallel , with an asymptotic temperature dependence

$$\xi_\parallel \sim (-t)^{-\nu_\parallel}. \quad (2.3)$$

According to Eq. (1.3) the correlation-length exponents satisfy the relation $\nu_\parallel = z\nu_\perp$. Going through the transition point by varying h at $t = 0$ leads to a similar behavior with $-t$ replaced by h in Eqs. (2.2) and (2.3), while the corresponding critical exponents are ν_\perp^h and ν_\parallel^h , respectively.

Now using the scaling hypothesis for strongly anisotropic systems²³ we can write the following relation for the singular part of the bulk free-energy density:

$$f(t, h, L) = b^{-(d-1)z+1} f(tb^{1/\nu_\perp}, hb^{1/\nu_\perp^h}, L/b), \quad (2.4)$$

when lengths are rescaled by a factor $b > 1$. By derivation one obtains a similar scaling relation for the bulk order parameter,

$$m_b(t, h, L) = \frac{\partial f}{\partial h} = b^{-[(d-1)z+1]+1/\nu_\perp^h} m_b(tb^{1/\nu_\perp}, hb^{1/\nu_\perp^h}, L/b), \quad (2.5)$$

and for the excess internal energy per degree of freedom,

$$\Delta u(t, h, L) = u(t, h, L) - u(0, 0, \infty) = \frac{\partial f}{\partial t} = b^{-[(d-1)z+1]+1/\nu_\perp} \Delta u(tb^{1/\nu_\perp}, hb^{1/\nu_\perp^h}, L/b). \quad (2.6)$$

Since the first-order transition is accompanied by a magnetization jump and a finite latent heat, both $m_b(t, h, L)$ and $\Delta u(t, h, L)$ approach a scale-independent, finite limit when $L \rightarrow \infty$. Thus Eqs. (2.5) and (2.6) lead to the scaling relations

$$\nu_\perp = \nu_\perp^h = \frac{1}{(d-1)z+1}. \quad (2.7)$$

One may notice that in the case of isotropic scaling, i.e., with $z = 1$, we recover the result of the DFP in Eq. (1.2).

For the susceptibility $\chi = \partial^2 f / \partial h^2$ and the specific heat $c_v = \partial^2 f / \partial t^2$, using the scaling relation in Eq. (2.4), we obtain

$$\begin{aligned} \chi(t, h = 0, L) &= t^{-\gamma_D} \tilde{\chi}_1(Lt^{\nu_\perp}) = L^{(d-1)z+1} \tilde{\chi}_2(Lt^{\nu_\perp}) \\ c_v(t, h = 0, L) &= t^{-\alpha_D} \tilde{c}_{v1}(Lt^{\nu_\perp}) = L^{(d-1)z+1} \tilde{c}_{v2}(Lt^{\nu_\perp}), \end{aligned} \quad (2.8)$$

with the DFP exponents γ_D and α_D in Eq. (1.1). The scaling functions behave as $\tilde{\chi}_1(y) \sim \tilde{c}_{v1}(y) \sim y^{(d-1)z+1}$ and $\tilde{\chi}_2(y) \sim \tilde{c}_{v2}(y) = \text{const}$ as $y \rightarrow 0$. Thus, *in a finite system*, when approaching the transition point, one can observe the development of a singularity with the DFP exponents in Eq. (1.1). However, in the thermodynamic limit $L \rightarrow \infty$, this singularity transforms into a δ function as it should at a first-order transition point. Indeed the temperature range where the surface can influence the behavior of the bulk is limited to $\Delta t \sim L^{-1/\nu_\perp}$, so that $\Delta t \chi(t = 0, h = 0, L) \approx 1$, and in this way $\chi(t, h = 0, L)$ —and similarly $c_v(t, h = 0, L)$ —is a representation of the δ function as $L \rightarrow \infty$. On the other hand, *at the transition point* the response functions show a power-law finite-size dependence, with the same critical exponent $(d-1)z+1$ as given in Eq. (2.8) and which should be measurable in finite samples.

For the correlation lengths one can similarly write the scaling relations

$$\begin{aligned} \xi_\perp(t, h, L) &= b \xi_\perp(tb^{1/\nu_\perp}, hb^{1/\nu_\perp^h}, L/b), \\ \xi_\parallel(t, h, L) &= b^z \xi_\parallel(tb^{1/\nu_\perp}, hb^{1/\nu_\perp^h}, L/b), \end{aligned} \quad (2.9)$$

from which the temperature (field) dependence in Eqs. (2.2) and (2.3) follows by taking the length scale as $b = t^{-\nu_\perp}$ ($b = h^{-\nu_\perp^h}$).

We close this section with a similar analysis of the singular behavior at the surface. For the singular part of the surface free energy per degree of freedom we write the scaling relation

$$\begin{aligned} f_1(t, h, h_1, L) \\ = b^{-(d-1)z} f_1(tb^{1/\nu_\perp}, hb^{1/\nu_\perp^h}, h_1 b^{(d-1)z-x_1}, L/b), \end{aligned} \quad (2.10)$$

where a surface ordering field h_1 with anomalous scaling dimension x_1 has been included. For the surface order parameter $m_1 = \partial f_1 / \partial h_1$, Eq. (2.10) leads to the following scaling behavior:

$$m_1(L) \sim L^{-x_1}, \quad m_1(t) \sim t^{x_1 \nu_\perp}. \quad (2.11)$$

Comparing Eqs. (2.2) and (2.11) we obtain

$$\beta_1 = x_1 \nu_\perp. \quad (2.12)$$

Taking other derivatives of f_1 one obtains similar scaling relations for the surface susceptibility $\chi_{1,1} = \partial^2 f_1 / \partial h_1^2$, for the excess surface order parameter $m_s = \partial f_1 / \partial h$, etc.

To conclude this section, let us remark that at a first-order transition point which is accompanied by SID, the bulk singularities in finite systems involve the anisotropy exponent z and the dimension d of the system whereas the surface singularities involve a new exponent x_1 . In the following section our scaling assumptions are confronted with analytical and numerical results on specific models.

III. THE TWO-DIMENSIONAL POTTS MODEL IN THE LARGE- q LIMIT

We start with the Hamiltonian of the classical q -state Potts model on the square lattice,¹⁹

$$\begin{aligned} -\beta H &= \sum_{k=-\infty}^{\infty} \sum_{l=1}^L K_1(l) [\delta(s_{l,k+1} - s_{l,k}) - 1] \\ &+ \sum_{k=-\infty}^{\infty} \sum_{l=1}^{L-1} K_2(l) \left[\delta(s_{l+1,k} - s_{l,k}) - \frac{1}{q} \right], \end{aligned} \quad (3.1)$$

where $s_{l,k} = 1, 2, \dots, q$ is a q -state Potts variable defined modulo q at site (l, k) . The vertical [horizontal] couplings $K_1(l)$ [$K_2(l)$] are ferromagnetic and may depend on the horizontal position l . Constant terms have been added in order to simplify some expressions in the following. The transfer operator T has matrix elements

$$\begin{aligned} \langle s|T|s' \rangle &= \langle s|U|s \rangle \langle s|V|s' \rangle, \\ \langle s|U|s \rangle &= \exp \left\{ \sum_{l=1}^{L-1} K_2(l) \left[\delta(s_{l+1} - s_l) - \frac{1}{q} \right] \right\}, \\ \langle s|V|s' \rangle &= \exp \left\{ \sum_{l=1}^L K_1(l) [\delta(s'_l - s_l) - 1] \right\}, \end{aligned} \quad (3.2)$$

between the Potts states $|s\rangle$ and $|s'\rangle$ associated with two successive rows k and $k+1$. Let us associate with each site l along a row the Potts operators Ω_l and M_l such that²⁴

$$\begin{aligned} \Omega_l |s_l\rangle &= \exp\left(i\frac{2\pi}{q}s_l\right) |s_l\rangle, \quad \Omega_l^\dagger = \Omega_l^{-1}, \\ M_l |s_l\rangle &= |s_l + 1\rangle, \quad M_l^\dagger = M_l^{-1}. \end{aligned} \quad (3.3)$$

Thus Ω_l is diagonal in the basis of the Potts states whereas M_l is a ladder operator. On the same site, they satisfy the commutation rules

$$\begin{aligned} M_l \Omega_l &= \exp\left(-i\frac{2\pi}{q}\right) \Omega_l M_l, \\ M_l^\dagger \Omega_l &= \exp\left(i\frac{2\pi}{q}\right) \Omega_l M_l^\dagger, \end{aligned} \quad (3.4)$$

and commute on different sites. Making use of the identity

$$\delta(s_{l+1} - s_l) = \frac{1}{q} \sum_{p=0}^{q-1} \exp\left[i\frac{2p\pi}{q}(s_{l+1} - s_l)\right], \quad (3.5)$$

the diagonal operator U can be written as

$$U = \exp\left\{\sum_{l=1}^{L-1} \frac{K_2(l)}{q} \sum_{p=1}^{q-1} (\Omega_l \Omega_{l+1}^\dagger)^p\right\}. \quad (3.6)$$

In Eq. (3.2) the diagonal matrix element $\langle s|V|s\rangle$ is equal to 1. When the two states $|s\rangle$ and $|s'\rangle$ differ only on site l , we have $\langle s|V|s'\rangle = \exp[-K_1(l)]$. Thus one may write the nondiagonal part of the transfer operator as

$$V = 1 + \sum_{l=1}^L \exp[-K_1(l)] \sum_{p=1}^{q-1} M_l^p + \dots, \quad (3.7)$$

where the ellipsis stands for higher-order terms involving products of exponentials coming from different sites.

In the extreme anisotropic limit²² where $K_1(l) \rightarrow \infty$, $K_2(l) \rightarrow 0$, and $\vartheta \rightarrow 0$ in such a way that the ratios

$$J_l = \frac{K_2(l)}{\vartheta}, \quad \Gamma_l = q \frac{\exp[-K_1(l)]}{\vartheta} \quad (3.8)$$

remain finite, the operators in Eqs. (3.6) and (3.7) are now given by

$$\begin{aligned} U &= 1 + \vartheta \sum_{l=1}^{L-1} \frac{J_l}{q} \sum_{p=1}^{q-1} (\Omega_l \Omega_{l+1}^\dagger)^p + O(\vartheta^2), \\ V &= 1 + \vartheta \sum_{l=1}^L \frac{\Gamma_l}{q} \sum_{p=1}^{q-1} M_l^p + O(\vartheta^2). \end{aligned} \quad (3.9)$$

To first order in ϑ , U and V commute and the transfer operator can be rewritten as the evolution operator

$T = \exp(-\vartheta \mathcal{H})$ for the infinitesimal Euclidian time step ϑ . According to Eqs. (3.2) and (3.9), the quantum Potts Hamiltonian takes the following form:

$$\mathcal{H} = - \sum_{l=1}^{L-1} \frac{J_l}{q} \sum_{p=1}^{q-1} (\Omega_l \Omega_{l+1}^\dagger)^p - \sum_{l=1}^L \frac{\Gamma_l}{q} \sum_{p=1}^{q-1} M_l^p. \quad (3.10)$$

Dual operators which satisfy the Potts algebra in Eq. (3.4) are defined as follows:

$$\begin{aligned} \widehat{M}_l &= \Omega_{l-1} \Omega_l^\dagger \quad (l = 2, L), \\ \widehat{M}_1 &= \Omega_1^\dagger, \\ \widehat{\Omega}_l &= \prod_{i=0}^{L-l-1} M_{l+i} M_{l+i+1}^\dagger \quad (l = 1, L-1), \\ \widehat{\Omega}_L &= M_L. \end{aligned} \quad (3.11)$$

Under the duality transformation the Hamiltonian in Eq. (3.10) is changed into

$$\mathcal{H} = - \sum_{l=2}^L \frac{J_{l-1}}{q} \sum_{p=1}^{q-1} \widehat{M}_l^p - \sum_{l=1}^{L-1} \frac{\Gamma_l}{q} \sum_{p=1}^{q-1} (\widehat{\Omega}_l \widehat{\Omega}_{l+1}^\dagger)^p - \frac{\Gamma_L}{q} \sum_{p=1}^{q-1} \widehat{\Omega}_L^p. \quad (3.12)$$

Having fixed boundary conditions with $s_L = 1$ amounts to have a vanishing transverse field Γ_L , which eliminates the last anomalous term in the dual Hamiltonian. The coupling J_{l-1} is transformed into a transverse field acting on the Potts state at l while the transverse field Γ_l becomes a coupling between Potts states at l and $l+1$. It follows that the original system with free-boundary conditions at $l = 1$ and fixed-boundary conditions at $l = L$ is transformed into a dual system with fixed-boundary conditions at $l = 1$ and free-boundary conditions at $l = L$. The Hamiltonian is strictly self-dual when $\Gamma_l = J_l$ either for homogeneous couplings $\Gamma = J$ or, with inhomogeneous couplings, when the sequence is symmetric. Then the self-duality point $J_l = \Gamma_l$ corresponds to the critical point.

In order to study the effect of a homogeneous longitudinal magnetic field, the Hamiltonian in Eq. (3.10) can be completed by the diagonal field term $-(h/\sqrt{q}) \sum_{l=1}^{L-1} [q\delta(s_l - 1) - 1]/(q-1)$.

In the calculations we consider the behavior of the system in the vicinity of the self-duality point, taking the parametrization

$$J_l = \Gamma_l \left(1 - \frac{t}{\sqrt{q}}\right), \quad (3.13)$$

where t plays the same role as the temperature in the classical model: for $t > 0$ ($t < 0$) we are in the bulk paramagnetic (ferromagnetic) phase with a vanishing (non-vanishing) order parameter. The local order parameter, i.e., the magnetization profile at site l , is defined as

$$m_l = \frac{q\langle 0|\delta(s_l - 1)|0\rangle - 1}{q - 1}, \quad (3.14)$$

where $|0\rangle$ is the ground-state eigenvector of \mathcal{H} . On the other hand, the free-energy density of the 2D classical

model is proportional to the ground-state energy per site, $e_0 = \langle 0|\mathcal{H}|0\rangle$.²²

In the large- q limit one may use a systematic expansion in powers of $1/\sqrt{q}$. To leading order the following eigenfunctions are degenerate:

$$\begin{aligned} |\psi_1\rangle &= |11\dots 11\rangle, \\ |\psi_2\rangle &= \frac{1}{q^{1/2}}(|21\dots 11\rangle + |31\dots 11\rangle + \dots + |q1\dots 11\rangle), \\ |\psi_3\rangle &= \frac{1}{q}[|321\dots 11\rangle + |421\dots 11\rangle + \dots + |q(q-1)1\dots 11\rangle], \\ |\psi_4\rangle &= \frac{1}{q^{3/2}}[|4321\dots 11\rangle + |5321\dots 11\rangle + \dots + |q(q-1)(q-2)1\dots 11\rangle], \\ &\vdots \\ |\psi_L\rangle &= \frac{1}{q^{(L-1)/2}}[|L\dots 4321\rangle + \dots + |q(q-1)(q-L)\dots(q-L+2)1\rangle], \end{aligned} \quad (3.15)$$

all having the same diagonal contribution $\langle \psi_i|\mathcal{H}|\psi_i\rangle = -\sum_{l=1}^{L-1} J_l = -\sum_{l=1}^{L-1} \Gamma_l$, where we made use of Eq. (3.13).

This degeneracy is lifted to the next order in $1/\sqrt{q}$ and the secular problem is governed by the operator

$$\tilde{\mathcal{H}} = -\frac{1}{\sqrt{q}} \begin{pmatrix} 0 & \Gamma_1 & & & 0 \\ \Gamma_1 & t\Gamma_1 - h & & & \\ & \Gamma_2 & \sum_{l=1}^2 (t\Gamma_l - h) & & \\ & & \Gamma_3 & & \\ & & \Gamma_3 & \sum_{l=1}^3 (t\Gamma_l - h) & \ddots \\ & & & \ddots & \ddots & \Gamma_{L-1} \\ 0 & & & & \Gamma_{L-1} & \sum_{l=1}^{L-1} (t\Gamma_l - h) \end{pmatrix}, \quad (3.16)$$

up to a constant term $-\sum_{l=1}^{L-1} \Gamma_l - (L-1)h/\sqrt{q}$. One may notice that for the homogeneous problem with $\Gamma_l = \Gamma$, the temperature and longitudinal field play the same role since we have the symmetry $t\Gamma \leftrightarrow -h$. The ground-state eigenvector of \mathcal{H} is given by the linear combination

$$|0\rangle = \sum_{i=1}^L v_i |\psi_i\rangle, \quad (3.17)$$

where v_i are the components of the leading eigenvector of $-\tilde{\mathcal{H}}$ in Eq. (3.16). Making use of Eqs. (3.14) and (3.15) we obtain the magnetization profile as

$$m_l = \sum_{i=1}^l |v_i|^2, \quad (3.18)$$

in the large- q limit. In particular the surface magnetization is given by $m_1 = |v_1|^2$ and the bulk magnetization is defined as $m_b = m_{L/2}$.

The perpendicular correlation length ξ_\perp gives the width of the interface region and, in the ordered phase, it can be defined through the relation

$$m_l|_{l=\xi_\perp} = \frac{1}{2}. \quad (3.19)$$

On the other hand, the parallel correlation length ξ_\parallel of the 2D classical model is related to the imaginary time spin-spin correlation function $G_l(\tau)$ of the quantum model. The long-time behavior of $G_l(\tau)$ has the asymptotic form

$$G_l(\tau) = \langle 0|\delta[s_l(0) - s_l(\tau)]|0\rangle \sim \exp(-\tau\Delta), \quad (3.20)$$

where Δ is the gap at the top of the spectrum of $-\tilde{\mathcal{H}}$. Since $\Delta \sim 1/\xi_\parallel$, one obtains information about the behavior of the correlations in the 2D classical system from the scaling properties of the spectrum of the Hamiltonian.²²

IV. SURFACE-INDUCED DISORDER IN REGULAR AND QUASIPERIODIC LATTICES

A. Solution on the regular lattice

For homogeneous interactions, i.e., when $\Gamma_l = \Gamma$, the complete solution of the Hamiltonian in Eq. (3.16) has

been given in Ref. 11. The critical exponents associated with the correlations parallel and perpendicular to the surface are given by

$$\nu_{\perp} = \nu_{\perp}^h = \frac{1}{3}, \quad \nu_{\parallel} = \nu_{\parallel}^h = \frac{2}{3}, \quad z = 2. \quad (4.1)$$

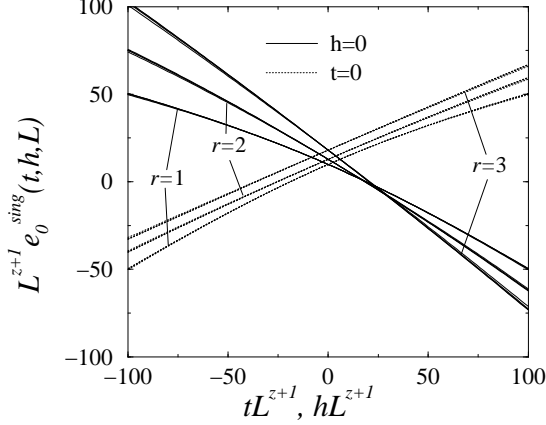


FIG. 1. Scaling plot of the singular part of the bulk energy density of the quantum Potts chain in the large- q limit for the regular ($r = 1$) and the Fibonacci lattice ($r = 2, 3$). The lines for finite systems with sizes $L = 89, 233, 610$, and 1597 are practically indistinguishable.

For the surface magnetization one obtains

$$x_1 = 3, \quad \beta_1 = 1. \quad (4.2)$$

First, one may notice that conventional scaling relations in Eq. (2.12) and below Eq. (2.3) are satisfied. More importantly, the relations in Eq. (2.7), which are a consequence of the discontinuous behavior in the bulk, are also satisfied.

Let us now consider the scaling of the free-energy density in Eq. (2.4). For the quantum chain it corresponds to the singular part of the ground-state energy density, $e_0^{\text{sing}}(t, h, L) = e_0(t, h, L) - e_0(0, 0, \infty)$, with the following finite-size scaling behavior:²⁵

$$e_0^{\text{sing}}(t, h, L) = L^{-(z+1)} \tilde{e}_0(tL^{z+1}, hL^{z+1}). \quad (4.3)$$

According to analytical results [see Eq. (26) in Ref. 11] this relation is indeed satisfied for the homogeneous system with $z = 2$. The numerical results for the scaling functions are shown in Fig. 1. They agree with the result of a perturbation expansion $\tilde{e}_0(y, 0) = \pi^2 - y/2 + O(y^3)$ to linear order. The scaling form of the magnetization profile in Eq. (2.5) is given by

$$m_l(t, h, L) = m_{l/L}(tL^{z+1}, hL^{z+1}). \quad (4.4)$$

It is presented in Fig. 2 for $h = 0$ and $t < 0$, $t > 0$, and $t = 0$. In the latter case the asymptotic scaling form is given by

$$m_{l/L}(0, 0) = \frac{l}{L} - \frac{1}{2\pi} \sin\left(\frac{2\pi l}{L}\right). \quad (4.5)$$

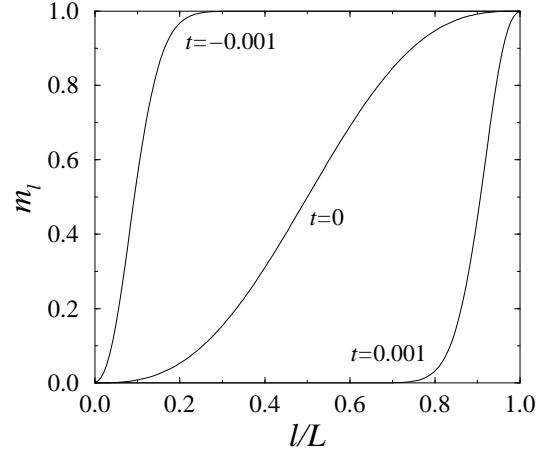


FIG. 2. Magnetization profiles of the homogeneous system with size $L = 144$ at different temperatures for free- and fixed-boundary conditions. The critical profile ($t = 0$) is the analytical result of Eq. (4.5). The interface for $t < 0$ ($t > 0$) is localized at the free (fixed) boundary.

In the ordered regime one can identify the interface region with width $\xi_{\perp} \sim t^{-1/(1+z)}$ near the surface at $l = 1$. In the high-temperature phase the interface has a width $\bar{\xi}_{\perp}$. It is localized near the ordered surface at $l = L$. The two widths are related through $\bar{\xi}_{\perp}(t) = \xi_{\perp}(-t)$, $t > 0$.

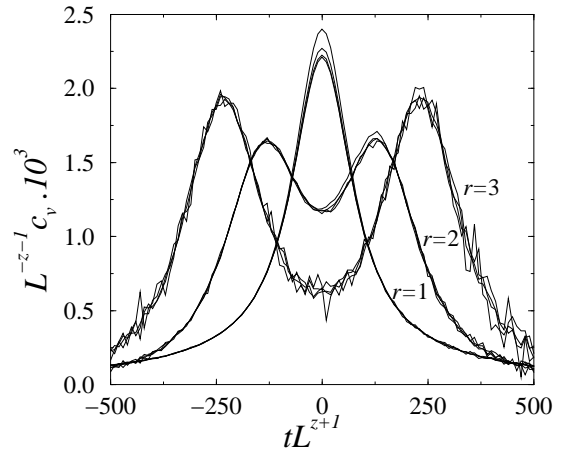


FIG. 3. Scaling plot of the specific heat of the quantum Potts chain in the large- q limit for the regular ($r = 1$) and the Fibonacci lattice ($r = 2, 3$). The lines are for finite systems with sizes $L = 89, 233, 610$, and 1597 . For the Fibonacci lattice a double-peak structure is obtained.

According to Eq. (4.3), the specific heat of the system, $c_v \sim \partial^2 e_0 / \partial t^2$, diverges with L as $c_v \sim L^3$ at the transition point, a behavior which is compatible with Eq. (2.8) with $z = 2$. Outside the transition point the scaling function has been calculated numerically and is shown in Fig. 3.

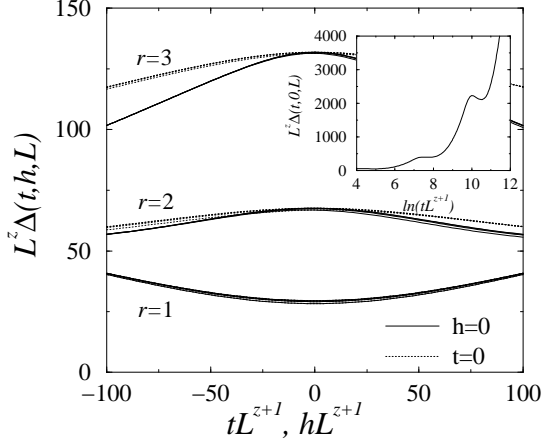


FIG. 4. Scaling plot of the energy gap of the quantum Potts chain in the large- q limit for the regular ($r = 1$) and the Fibonacci lattice ($r = 2, 3$). The lines for finite systems with sizes $L = 89, 233, 610$, and 1597 indicate a good data collapse. The inset shows log-periodic oscillations of the scaled gap at larger values of the scaling variable for $r = 2$ and $L = 89$.

Finally, we checked the scaling relation for the parallel correlation length in Eq. (2.9). It is related to the scaling behavior of the gap of the quantum Potts chain which is given by

$$\Delta(t, h, L) = L^{-z} \tilde{\Delta}(tL^{z+1}, hL^{z+1}). \quad (4.6)$$

The results of numerical calculations for the scaling function $\tilde{\Delta}(y, 0) = \tilde{\Delta}(0, -y)$ are shown in Fig. 4. They agree with the analytical result $\tilde{\Delta}(0, 0) = 3\pi^2$ [see Eq. (21) in Ref. 11].

B. Fibonacci lattice

The 1D Fibonacci lattice is composed of two units A and B , and starting from A the sequence is generated through substitutions $A \rightarrow AB$ and $B \rightarrow A$. The couplings or transverse fields on the lattice are also two valued, Γ_A and Γ_B , depending on the letter in the sequence at the given position. The strength of the quasiperiodic perturbation is measured by the ratio $r = \Gamma_B / \Gamma_A$. It has been noticed in Refs. 26 and 27, that the 2D layered Fibonacci lattice and the 2D Penrose quasilattice have a similar structure. On the Penrose lattice, starting from a straightlike surface, two different types of parallel layers can be identified, which are distributed according to the

Fibonacci sequence. Consequently the SID phenomenon studied here on the layered Fibonacci lattice should behave in the same way on the Penrose lattice.

Considering the Potts model in the large- q limit²⁸ the effective Hamiltonian in Eq. (3.16) at the transition point $t = h = 0$ takes the form of a 1D quasiperiodic Schrödinger Hamiltonian, the properties of which have been extensively studied.²⁹ In particular, the scaling properties of the spectrum of $\tilde{\mathcal{H}}$ at special points, such as at the edge of the spectrum, are exactly known.³⁰

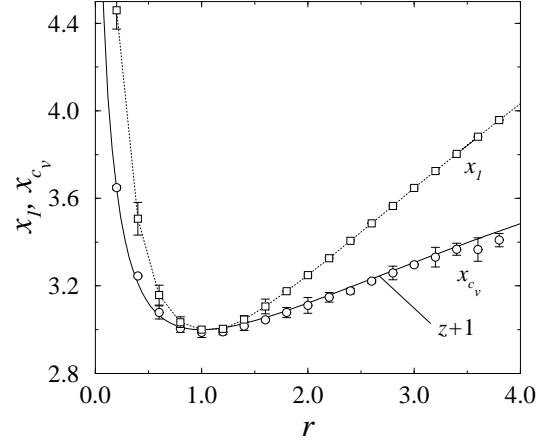


FIG. 5. Finite-size-scaling exponents of the specific heat x_{c_v} and surface magnetization x_1 , as a function of the amplitude ratio r . The solid line represents the exact scaling result $x_{c_v} = z + 1$ with z given by Eqs. (4.8) and (4.9). The dotted line is a guide to the eye.

They are relevant for the strongly anisotropic scaling in our problem. The integrated density of states $D(\Delta E)$, measured from the top of the spectrum of $-\tilde{\mathcal{H}}$ has the scaling property³⁰

$$D(\Delta E) \sim |\Delta E|^\sigma, \quad \Delta E \rightarrow 0. \quad (4.7)$$

Here

$$\frac{1}{\sigma} = \frac{\ln \lambda}{\ln \phi^2}, \quad (4.8)$$

where $\phi = (1 + \sqrt{5})/2$ is the golden-mean ratio, $\lambda = \{8J - 1 + [(8J - 1)^2 - 4]^{1/2}\}/2$ with $J = [3 + (25 + 16I)^{1/2}]/8$ and $I = (r + r^{-1})^2/4$.

A relation between the exponent σ and the anisotropy exponent z can be obtained by noticing the scaling relation for the integrated density of states $D' = D(\Delta E') = bD(\Delta E)$ when lengths are rescaled as $L' = L/b$, since $D(\Delta E)$ is the number of states per unit length. Using also the scaling relation for the gaps $\Delta E' = b^z \Delta E$, as given in Eq. (4.6), we arrive at the result

$$z = \frac{1}{\sigma}. \quad (4.9)$$

Consequently, the anisotropy exponent of the Potts model on the Fibonacci lattice is exactly known. Thus we can check the bulk scaling relations derived for SID, which contains only the anisotropy exponent z as a parameter. The scaling behavior of the energy density in Eq. (4.3) with varying temperature and field is illustrated in Fig. 1. An excellent data collapse is obtained for the lengths indicated, i.e., for Fibonacci numbers F_n with an odd index n . A different scaling function is obtained for n even. The scaling functions corresponding to the temperature and field perturbations are no longer related through inversion, as they were for the homogeneous problem.

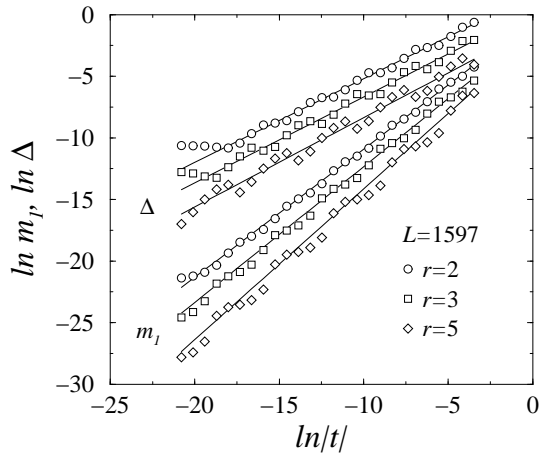


FIG. 6. Temperature dependence of the gap (Δ) and the surface magnetization (m_l) of the Potts model on the Fibonacci lattice with $L = 1597$ for different values of r , on a double-logarithmic scale. The numerically calculated points, which show log-periodic oscillations, are compared to asymptotic scaling results shown by straight lines. The slope of the lines are $\nu_{\parallel} = z/(z+1)$ and $\beta_1 = x_1/(z+1)$, for Δ and m_l , respectively, where x_1 is taken from Fig. 5. Deviations from the linear behavior at small $|t|$ values are due to finit-size effects. Some sets of data were shifted vertically in order to improve the legibility.

We have also studied the finite-size scaling behavior of the specific heat at the transition point which is given by $c_v(t=0, h=0, L) \sim L^{x_{c_v}}$ and, according to Eq. (2.8), $x_{c_v} = z+1$. The exponents $x_{c_v}(r)$ were obtained through the extrapolation of two-point approximants using the Bulirsch-Stoer (BS) algorithm.^{31,32} As shown in Fig. 5 this scaling relation is indeed satisfied in the whole range of amplitude ratio r investigated.

The scaling form of the specific heat in Eq. (2.8) is shown in Fig. 3. For the Fibonacci lattice the scaling function around $t = 0$ has a double peak structure with a distance between the peaks increasing with r .

The finite-size scaling behavior of the energy gap given in Eq. (4.6) is tested numerically in Fig. 4 as a function of temperature and field. The unexpected maximum of the scaled gap at the transition point can be attributed

to the presence of log-periodic oscillations, as shown in the inset for larger values of the scaling variable tL^{z+1} . Outside the transition point, the gap remains finite with an asymptotic temperature dependence $\Delta(t) \sim t^{\nu_{\parallel}}$, with $\nu_{\parallel} = z/(z+1)$. The numerical results for the temperature dependence, which is perturbed by log-periodic oscillations, is shown in Fig. 6 for different values of r .

Next we present the results about the surface scaling properties of the Potts model on the Fibonacci lattice. The determination of the order parameter, even at the surface, requires knowledge of the ground-state eigenvector of \mathcal{H} as shown in Eq. (3.18). With lack of an exact knowledge of this eigenvector we calculated numerically the surface magnetization at the transition point as a function of the size of the system, and the scaling exponent x_1 , defined in Eq. (2.11), was obtained through the extrapolation of two-point approximants using the BS algorithm. It is shown in Fig. 5 as a function of r . The surface magnetization was also calculated as a function of t for $L = 1597$ in order to check the scaling relation in Eq. (2.12) for the exponent β_1 . The results are shown in Fig. 6.

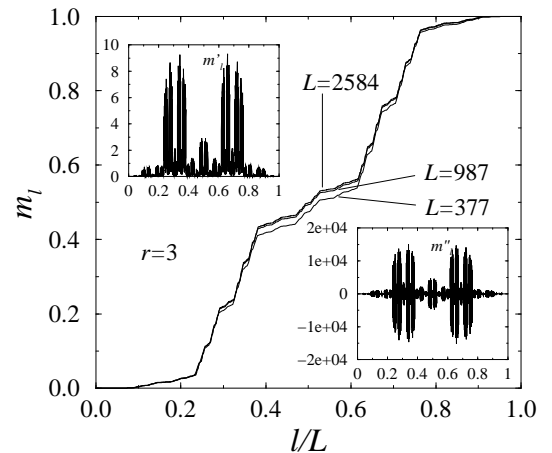


FIG. 7. Magnetization profile of the quantum Potts chain at the transition point calculated on finite Fibonacci lattices with fixed- and free-boundary conditions. In the insets the first and second finite differences are taken for $L = 2584$.

We close this section by presenting in Fig. 7 the magnetization profiles calculated at the transition point on finite Fibonacci lattices. At first sight the shape of the curves for different lengths looks similar; however, a closer inspection shows that with increasing size there are more and more points where a steplike behavior develops. To look for a possible nonanalytical behavior of the curve in the thermodynamic limit we have calculated the finite size differences $\Delta_1 m_l = L(m_{l+1} - m_{l-1})/2$ and $\Delta_2 m_l = L^2(m_{l+1} + m_{l-1} - 2m_l)$. As seen in the insets of Fig. 7, the derivatives show a self-similar, multifractal structure. With increasing size L the heights of the peaks are increasing, indicating divergent first and second derivatives. Consequently m_l/L is an example of

a physical observable with nonanalytical mathematical properties.

V. DISCUSSION

In this paper we have presented a scaling picture for bulk first-order transitions associated with SID, i.e., with a continuous surface transition. We have shown that fluctuations of the interface separating the ordered (bulk) and disordered (surface) regions govern the scaling behavior of bulk quantities. Power-law singularities are present and the bulk free-energy density shows a strongly anisotropic scaling behavior at the first-order transition point, which can be associated with an anisotropic DFP.

The discontinuous nature of the bulk transition fixes the form of the scaling exponents, which can all be expressed in terms of the anisotropy exponent z and the dimension of the system. Also the functional form of the scaling functions is particular. For example, response functions at the transition point have a power-law-type size-dependent peak, from which a δ -function singularity develops in the thermodynamic limit.

The scaling picture for SID has been tested on the 2D Potts model in the large- q limit, both on the regular lattice and on the layered Fibonacci lattice (the latter is related to the 2D Penrose quasilattice). For the Fibonacci lattice the anisotropy exponent z varies continuously with the amplitude ratio of the aperiodicity in an exactly known way. The study of the associated variation of other scaling exponents provides us with a stronger test of the SID scaling relations.

The marginal nature of the quasiperiodic perturbation of the Fibonacci type should be explainable through a relevance-irrelevance criterion, like the Harris criterion¹³ for critical systems in the presence of quenched disorder.

For second-order transitions the relevance or irrelevance of aperiodic perturbations is generally related to the size dependence of the fluctuations of the sequence, which is measured by the wandering exponent ω . For a 1D variation, as considered in this paper, ω is defined through the cumulated deviation from the average³³

$$\Delta_{\Gamma}(L_n) = \sum_{l=1}^{L_n} (\Gamma_l - \bar{\Gamma}) \sim L_n^{\omega}, \quad (5.1)$$

where $\bar{\Gamma} = \lim_{L_n \rightarrow \infty} (1/L_n) \sum_{l=1}^{L_n} \Gamma_l$ is the average field and L_n is the length of the sequence after n substitutions (i.e., the Fibonacci number F_n). As shown in Refs. 34 and 35, for a thermal aperiodic perturbation, the crossover exponent at the fixed point of the pure system is $\varphi = 1 + \nu_{\perp}(\omega - 1)$, where ν_{\perp} is the perpendicular correlation length exponent of the pure system. Such a perturbation is relevant (irrelevant) when $\varphi > 0$ ($\varphi < 0$).

A naive application of this criterion to our problem, with $\nu_{\perp} = 1/3$ according to Eq. (4.1), leads to a marginal

value of the wandering exponent $\omega = -2$. Thus the perturbation should be relevant for the Fibonacci sequence with $\omega = -1$.

Actually, the self-dual form of the aperiodic perturbation considered in this work, with $J_l = \Gamma_l$ in Eq. (3.10), is weaker than a standard thermal perturbation for which, for example, J_l fluctuates aperiodically while Γ_l is kept constant.

In order to obtain a relevance-irrelevance criterion adapted to our problem, let us consider the form of the Hamiltonian matrix in Eq. (3.16) and compare the perturbation associated with a deviation t from the transition point, on the one hand, to the perturbation introduced by the aperiodic fluctuations on the other hand.

The temperature perturbation contributes to the diagonal elements by terms of the form

$$t \sum_{j=1}^k \Gamma_j = \bar{\Gamma} t k + t \sum_{j=1}^k (\Gamma_j - \bar{\Gamma}). \quad (5.2)$$

According to Eq. (5.1) when k is large the last term behaves as $t k^{\omega}$ and may be neglected since the wandering exponent is always smaller than 1. Taking the average at a length scale $L \gg 1$ of the leading contribution to Eq. (5.2), one obtains the following estimate for the temperature perturbation:

$$\delta_t(L) = \frac{\bar{\Gamma} t}{L} \sum_{k=1}^{L-1} k \sim t L. \quad (5.3)$$

The aperiodic fluctuations contribute mainly to the off-diagonal terms and using Eq. (5.1), their mean value at the length scale L is given by

$$\delta_{\Gamma}(L) = \frac{1}{L} \Delta_{\Gamma}(L) \sim L^{\omega-1}. \quad (5.4)$$

The appropriate length scale is the perpendicular correlation length ξ_{\perp} and the relevance of the aperiodic perturbation depends on the value of the ratio

$$\frac{\delta_{\Gamma}(\xi_{\perp})}{\delta_t(\xi_{\perp})} \sim t^{1+\nu_{\perp}(\omega-2)}, \quad (5.5)$$

where we used Eq. (2.2). Thus for self-dual aperiodic perturbations the crossover exponent is

$$\varphi_{\text{sd}} = 1 + \nu_{\perp}(\omega - 2). \quad (5.6)$$

It follows that with $\nu_{\perp} = 1/3$ such perturbations are marginal when $\omega = -1$, in agreement with our results for the Fibonacci lattice.

Finally, let us briefly mention that we have also studied the effect of an aperiodic perturbation following the period-doubling sequence.³⁶ This sequence is generated through the substitutions $A \rightarrow AB, B \rightarrow AA$, and its wandering exponent is $\omega = 0$. According to Eq. (5.6) this perturbation is relevant at the first-order transition point of the q -state Potts model. Indeed, using the results of an exact renormalization group method in Ref. 16,

the anisotropy exponent is found to be formally infinite. More precisely the correlation lengths are related through

$$\ln \xi_{\parallel} \sim \xi_{\perp}^{\mu}, \quad (5.7)$$

where $\mu = 1/2$ for the period-doubling sequence.³⁷

ACKNOWLEDGMENTS

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- ¹ B. Nienhuis and N. Nauenberg, Phys. Rev. Lett. **35**, 477 (1975).
 - ² M. E. Fisher and A. N. Berker, Phys. Rev. B **26**, 2507 (1982).
 - ³ B. Nienhuis, A. N. Berker, E. K. Riedel, and M. Schick, Phys. Rev. Lett. **43**, 737 (1979).
 - ⁴ J. Sólyom and P. Pfeuty, Phys. Rev. B **24**, 218 (1981).
 - ⁵ R. Lipowsky, Phys. Rev. Lett. **49**, 1575 (1982).
 - ⁶ See S. Dietrich, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic, New York, 1988), Vol. 12, p. 1.
 - ⁷ R. Lipowsky, J. Appl. Phys. **55**, 2485 (1984).
 - ⁸ D. M. Kroll and G. Gompper, Phys. Rev. B **36**, 7078 (1987).
 - ⁹ G. Gompper and D. M. Kroll, Phys. Rev. B **38**, 459 (1988).
 - ¹⁰ H. Dosch, *Critical Phenomena at Surfaces and Interfaces*, Springer Tracts in Modern Physics, Vol. 126 (Springer, Berlin, 1992).
 - ¹¹ F. Iglói and E. Carlon, Phys. Rev. B **59**, 3783 (1999).
 - ¹² F. Iglói, I. Peschel, and L. Turban, Adv. Phys. **42**, 683 (1993).
 - ¹³ A. B. Harris, J. Phys. C **7**, 1671 (1974).
 - ¹⁴ C. Godreche, J. M. Luck, and H. J. Orland, J. Stat. Phys. **45**, 777 (1986); Y. Okabe and K. Nizeki, J. Phys. Soc. Jpn. **57**, 1536 (1988); E. S. Sørensen, M. V. Jarić, and M. Ronchetti, Phys. Rev. B **44**, 9271 (1991); Y. Okabe and K. Nizeki, J. Phys. A **23**, L733 (1990).
 - ¹⁵ F. Iglói and L. Turban, Phys. Rev. Lett. **77**, 1206 (1996).
 - ¹⁶ F. Iglói, L. Turban, D. Karevski, and F. Szalma, Phys. Rev. B **56**, 11 031 (1997).
 - ¹⁷ J. Hermisson, U. Grimm, and M. Baake J. Phys. A **30**, 7315 (1997).
 - ¹⁸ R. J. Baxter, J. Phys. C **6**, L445 (1973).
 - ¹⁹ For a review on the Potts model, see F. Y. Wu, Rev. Mod. Phys. **54**, 235 (1982).
 - ²⁰ M. Aizenman and J. Wehr, Phys. Rev. Lett. **62**, 2503 (1989).
 - ²¹ P. E. Berche, C. Chatelain, and B. Berche, Phys. Rev. Lett. **80**, 297 (1998).
 - ²² J. Kogut, Rev. Mod. Phys. **51**, 659 (1979).
 - ²³ K. Binder and L. S. Wang, J. Stat. Phys. **55**, 87 (1989).
 - ²⁴ L. Mittag and H. J. Stephen, J. Math. Phys. **12**, 441 (1971).
 - ²⁵ Actually, in the large- q limit, e_0^{sing} is to be understood as the singular part of $\sqrt{q}\langle 0|\mathcal{H}|0\rangle$ according to Eq. (3.16).
 - ²⁶ C. L. Henley and R. Lipowsky, Phys. Rev. Lett. **59**, 1679 (1987).
 - ²⁷ A. Garg and D. Levine, Phys. Rev. Lett. **59**, 1683 (1987).
 - ²⁸ Since the sequence is not symmetric, the Fibonacci Hamiltonian is only approximately self-dual. Nevertheless, the critical point remains located at $J_t = \Gamma_t$.
 - ²⁹ M. Kohmoto, L. P. Kadanoff, and C. Tang, Phys. Rev. Lett. **50**, 1870 (1983); S. Ostlund, R. Pandit, D. Rand, H. J. Schellnhuber, and E. D. Siggia, Phys. Rev. Lett. **50**, 1873 (1983).
 - ³⁰ M. Kohmoto, B. Sutherland, and C. Tang, Phys. Rev. B **35**, 1020 (1987).
 - ³¹ R. Bulirsch and J. Stoer, Numer. Math. **6**, 413 (1964).
 - ³² M. Henkel and G. Schütz, J. Phys. A **21**, 2617 (1988).
 - ³³ M. Queffélec, in *Substitutional Dynamical Systems-Spectral Analyses*, edited by A. Dold and B. Eckmann, Lecture Notes in Mathematics, Vol. 1294 (Springer, Berlin, 1987).
 - ³⁴ J. M. Luck, J. Stat. Phys. **72**, 417 (1993).
 - ³⁵ F. Iglói, J. Phys. A **26**, L703 (1993).
 - ³⁶ P. Collet and B. Eckmann, *Iterated Maps in the Interval as Dynamical Systems* (Birkhäuser, Boston, 1980).
 - ³⁷ Actually, the exact calculation of the exponent μ was done in Ref. 16 for a directed walk problem. The aperiodic modulation of the weights corresponds in the present problem to the two-letter substitutions obtained by replacing A by AA and B by AB in the period-doubling sequence. One expects the same critical behavior since the wandering exponent is not modified by this decoration of the sequence. This is supported by numerical data.